

Three-body correlations in the Nagaoka state on the square lattice

Jun-ichi Igarashi, Manabu Takahashi, and Tatsuya Nagao
Faculty of Engineering, Gunma University, Kiryu, Gunma 376-8515, Japan

A three-body scattering theory previously proposed by one of the present authors is developed to be applied to the saturated ferromagnetic state in the two-dimensional Hubbard model. The single-particle Green's function is calculated by taking account of the multiple scattering between two electrons and one hole. Several limiting cases are discussed and the relation to the variational principle is examined. The importance of the three-body correlation is demonstrated in comparison with the results of the ladder approximation. A possible phase boundary for the Nagaoka ground state is presented for the square lattice, which improves the previous variational results.

71.10.Fd, 71.28.+d, 75.30.Kz

I. INTRODUCTION

Electron correlations in narrow bands have attracted much attention after the discovery of high T_c cuprate superconductors. Since a thorough study of electron correlations is quite complicated in actual materials, we often use a simplified model to understand the essence of the effects. One of the most widely used models is the Hubbard model,¹⁻³ whose Hamiltonian is given by

$$H = -t \sum_{\langle i,j \rangle \sigma} a_{i\sigma}^\dagger a_{j\sigma} + \text{H.c.} + U \sum_i a_{i\uparrow}^\dagger a_{i\downarrow}^\dagger a_{i\downarrow} a_{i\uparrow}, \quad (1.1)$$

where $t > 0$ and $\langle i, j \rangle$ stands for the nearest neighbor pairs. Operator $a_{i\sigma}$ represents the annihilation of an electron with spin σ at site i .

In the low density of occupied electrons, the correlation effects on this model are exactly taken into account by considering the multiple scattering between two electrons. Using this low-density theory, Kanamori² studied the ferromagnetism of nickel metal (here holes are in low density). He found that the effective interaction between electrons is considerably reduced from the bare value U due to the correlated motion avoiding each other, and that the Stoner condition for ferromagnetism is strongly modified. In order to extend his theory to higher density, we need to include also the effects of the particle-hole multiple scattering, which describes the magnon excitation on the ferromagnetic ground state, and those of the electron-magnon interaction. Hertz and Edwards⁴ recognized the importance of the vertex correction, and determined the electron-magnon vertex by enforcing the Ward-Takahashi identity.⁵ However, it is impossible to determine the vertex on all points in the momentum-frequency space by the identity alone, and also it is unclear how to include the particle-particle multiple-scattering effect, which becomes important in the low density of electrons. One of the present author has proposed a theory^{6,7} which takes account of the multiple scattering between two electrons and one hole with the use of the Faddeev equation of the three-body problem.⁶⁻¹⁰ This theory naturally takes account of the particle-particle and particle-hole multiple-scattering channels on equal footing, and thereby it contains the effect interpreted as the vertex correction for the electron-magnon interaction.

The three-body scattering theory has a clear meaning of the three-body problem on the saturated ferromagnetic ground state, although it is applicable to the paramagnetic phase by deriving a similar integral equation to the Faddeev equation. In this paper, in order to make clear the physical meaning and the reliability of the approximation, we confine ourselves to the application to the two-dimensional Hubbard model in the context of the instability of the saturated ferromagnetic ground state. It has a nice property interpolating from the low-density limit to the half-filling limit, and satisfies the exact atomic limit¹ as previously proved.^{6,8} One of the present authors⁷ has already applied the three-body scattering theory to the one-dimensional Hubbard model in comparison with the exact solution, having calculated the spectral function for the single-particle Green's function. Later Ruckenstein and Schmitt-Rink⁸ have examined the same approach in comparison with other theories. However, the actual calculation in two dimensions has not been carried out yet. In this paper, we calculate the single-particle Green's function in two dimensions and determine the quasi-particle energy. We demonstrate the importance of the three-body correlation by comparison with the ladder approximation. We find that a low-energy scale for the quasi-particle energy, which is much smaller than its value of the ladder approximation, and that the mass enhancement factor is as large as ~ 10 in the strong coupling regime. We discuss several limiting cases for clarifying the approximation made. We also show that the

present theory satisfies the variational principle.⁹ This observation helps us to compare the present theory to other variational theories.

As regards the stability of saturated ferromagnetism, Nagaoka considered in his pioneering study the case of one hole in an otherwise half-filled band with $U = \infty$.^{11,12} He proved that the saturated ferromagnetism is realized as ground state on appropriate lattices due to gaining the kinetic energy of the hole. For two holes on a square lattice with $U = \infty$, Fang *et al.*¹³ found that the ground state is a singlet by exact diagonalizations for small clusters. Doucot and Wen¹⁴ found that a long-wave length twisted spin state has lower energy than the saturated ferromagnetic state. On the other hand, it has been noticed that finite-size effects are crucial and that closed-shell configurations (numbers of holes are 1, 5, 9, ...) favor ferromagnetism whereas open-shell configurations (numbers of holes are 2, 3, 4, 6, ...) tend to destabilize it.^{15,16} Quantum Monte Carlo results suggest no ferromagnetic phase for intermediate U ,^{15,17} but the cluster sizes used and the simulation temperatures are rather high. Therefore, for a thermodynamic concentration of holes, such considerations for a few holes do not serve as proper guides.

Another route to investigate the stability of the Nagaoka ground state is a variational study for the excitation energy with respect to overturning an up-spin electron and placing it on a down-spin band. Of course this approach gives only an upper limit for the ferromagnetic boundary. Roth¹⁸ was the first to discuss in detail the instability of the Nagaoka ground state with an approximate scheme equivalent to using a variational wave function. It is found superior to the Gutzwiller function, since it has more variational flexibility.¹⁹ The similar variational wave function was employed by Shastry, Krishnamurthy, and Anderson,²⁰ for discussing the instability of the Nagaoka ground state and the spin-wave stiffness. It was also used to calculate the spin-wave spectrum with general momentum in the $U = \infty$ limit by Basile and Elser²¹, and for finite U by Okabe.²² The softening of the spin-wave energy may set another condition for the instability of the Nagaoka state. These calculations leads to an instability for a finite concentration of holes even in the $U = \infty$ limit. Another interesting variational wave function is constructed by Richmond and Rickayzen,²³ who froze the motion of the down-spin electron and solved exactly the states for up-spin electrons under the static potential due to the down-spin electron (see Appendix B). This study merely leads to the conclusion that the Nagaoka state is always stable in the $U = \infty$ limit for any concentrations of holes. Recently, Hanish, Uhlig, and Müller-Hartman²⁴ analyzed Roth's wave function and its slight extension on various lattices, and calculated the phase diagram for the Nagaoka ground state. The present theory is shown to be equivalent to using a variational wave function similar to Roth's but assuming the most general form with the states containing one particle-hole pair. It is more flexible than that of Hanish *et al.*,²⁴ and thereby we obtain the phase diagram with a smaller area of the Nagaoka ground state than Hanish *et al.* This may serve as a measure of the accuracy of the present theory.

In Sec. II, the three-body scattering theory is formulated for the single-particle Green's function, and several limiting formulas are derived. The relation to the variational method is also discussed. In Sec. III, the numerical solution is presented for the square lattice. Section IV contains concluding remarks. In the Appendix A, the explicit solution of the Faddeev equation is derived in the $U = \infty$ limit, and in the Appendix B the method of Richmond and Rickayzen is adapted for numerical computations.

II. THREE-BODY SCATTERING THEORY

We briefly summarize the three-body scattering theory, and discuss several limiting formulas, which are useful to make clear the physical meaning of the approximation made. We also discuss the variational character of the theory.

A. The Green's function formalism

We start by assuming the saturated ferromagnetic ground state, where only up-spin states are occupied by electrons. No interaction is working between electrons with the same spin. Placing a down-spin electron into the system, we study its motion using the single-particle Green's function.

We make a perturbational expansion, where the Hartree-Fock energy is included into the unperturbed part. Thus the Hamiltonian is divided into two parts:

$$H = H_0 + H_1, \quad (2.1)$$

where

$$H_0 = \sum_{\mathbf{k}} [\epsilon_{\mathbf{k}} a_{\mathbf{k}\uparrow}^\dagger a_{\mathbf{k}\uparrow} + (\epsilon_{\mathbf{k}} + U n) a_{\mathbf{k}\downarrow}^\dagger a_{\mathbf{k}\downarrow}], \quad (2.2)$$

$$H_1 = \frac{U}{N} \sum_{\mathbf{p}_1 \mathbf{p}_2 \mathbf{q}} a_{\mathbf{p}_1 + \mathbf{q}\downarrow}^\dagger \left(a_{\mathbf{p}_2 - \mathbf{q}\uparrow}^\dagger a_{\mathbf{p}_2\uparrow} - \langle a_{\mathbf{p}_2 - \mathbf{q}\uparrow}^\dagger a_{\mathbf{p}_2\uparrow} \rangle \right) a_{\mathbf{p}_1\downarrow}. \quad (2.3)$$

Here N is the number of lattice sites and $\langle \dots \rangle$ denotes the average over the ground state. Momentum \mathbf{k} is defined in the first Brillouin zone, *i. e.*, $-\pi < k_x \leq \pi$ and $-\pi < k_y \leq \pi$ in units of $1/a$ with a being the nearest neighbor distance for the square lattice. The kinetic energy with momentum \mathbf{k} is given by $\epsilon_{\mathbf{k}} = -2t(\cos k_x + \cos k_y)$ for the square lattice. The occupied electron density n is defined by

$$n\delta_{\mathbf{q},\mathbf{0}} = \frac{1}{N} \langle \sum_{\mathbf{p}} a_{\mathbf{p}-\mathbf{q}\uparrow}^\dagger a_{\mathbf{p}\uparrow} \rangle. \quad (2.4)$$

The single-particle Green's function is defined by

$$G_\sigma(\mathbf{k}, t) = -i \langle T[a_{\mathbf{k}\sigma}(t) a_{\mathbf{k}\sigma}^\dagger(0)] \rangle, \quad (2.5)$$

where T represents the time ordering, and $a_{\mathbf{k}\sigma}(t) = \exp(i(H - \mu N_e)t) a_{\mathbf{k}\sigma} \exp(-i(H - \mu N_e)t)$ with μ and N_e being the chemical potential and the number operator of electrons. On the saturated ferromagnetic ground state, only the retarded part does not vanish with the down-spin electron, *i. e.*,

$$G_\downarrow(\mathbf{Q}, z) = -i \int_0^\infty \langle T[a_{\mathbf{Q}\downarrow}(t) a_{\mathbf{Q}\downarrow}^\dagger(0)] \rangle e^{izt} dt, \quad z = \omega + i\eta \quad (\eta \rightarrow 0^+). \quad (2.6)$$

The unperturbed Green's function is given by

$$G_\downarrow^{(0)}(\mathbf{Q}, z)^{-1} = z - \epsilon_{\mathbf{Q}} - Un + \mu, \quad (2.7)$$

with Un being the HF potential. The self-energy is defined by

$$G_\downarrow(\mathbf{Q}, z)^{-1} = G_\downarrow^{(0)}(\mathbf{Q}, z)^{-1} - \Sigma_\downarrow(\mathbf{Q}, z). \quad (2.8)$$

We sum up all the Feynman diagrams for the self-energy shown in Fig. 1, where only three lines of Green's function exist in the intermediate states. An important point is that the frequency sum in the intermediate states can be explicitly carried out, since the Green's function for the down-spin electron consists only of a retarded part. After the frequency sum, we obtain

$$\begin{aligned} \Sigma_\downarrow(\mathbf{Q}, z) = & \left(\frac{U}{N} \right)^2 \left\{ \sum_{\mathbf{p}\mathbf{q}} G_0(\mathbf{Q}, z; \mathbf{p}\mathbf{q}) + \sum_{\mathbf{p}\mathbf{q}\mathbf{q}'} G_0(\mathbf{Q}, z; \mathbf{p}\mathbf{q}) \frac{U}{N} G_0(\mathbf{Q}, z; \mathbf{p}\mathbf{q}') \right. \\ & \left. + \sum_{\mathbf{p}\mathbf{p}'\mathbf{q}} G_0(\mathbf{Q}, z; \mathbf{p}\mathbf{q}) \frac{-U}{N} G_0(\mathbf{Q}, z; \mathbf{p}'\mathbf{q}) + \dots \right\}, \end{aligned} \quad (2.9)$$

where

$$G_0(\mathbf{Q}, z; \mathbf{p}\mathbf{q}) = 1/(z - \epsilon_{\mathbf{Q}+\mathbf{p}-\mathbf{q}} - Un - \epsilon_{\mathbf{q}} + \epsilon_{\mathbf{p}} + \mu). \quad (2.10)$$

Hereafter \mathbf{p}, \mathbf{p}' are restricted inside the Fermi sphere, and \mathbf{q}, \mathbf{q}' are restricted outside the Fermi sphere.

We notice that Eq. (2.9) is equivalent to collecting up all the multiple-scattering processes between two particles and one hole. This three-body problem is exactly solvable by using the Faddeev equation.²⁵ We write down the Faddeev equation for the scattering matrix $T(z)$;

$$T(z) = T_1(z) + T_2(z), \quad (2.11)$$

with

$$\begin{pmatrix} T_1(z) \\ T_2(z) \end{pmatrix} = \begin{pmatrix} t_1(z) \\ t_2(z) \end{pmatrix} + \begin{pmatrix} 0 & t_1(z) \\ t_2(z) & 0 \end{pmatrix} G_0(z) \begin{pmatrix} T_1(z) \\ T_2(z) \end{pmatrix}. \quad (2.12)$$

Here $G_0(z)$ is a free propagator $1/(z - H_0)$, $t_1(z)$ is the particle-particle scattering matrix, and $t_2(z)$ is the particle-hole scattering matrix. All these quantities are represented within three-body states. As shown in Fig. 2, we introduce three-body states with total momentum \mathbf{Q} , which are written as

$$|\mathbf{Q}; \mathbf{p}\mathbf{q}\rangle \equiv a_{\mathbf{Q}+\mathbf{p}-\mathbf{q}\downarrow}^\dagger a_{\mathbf{q}\uparrow}^\dagger a_{\mathbf{p}\uparrow} |F\rangle. \quad (2.13)$$

Here $|F\rangle$ is the saturated ferromagnetic ground state. Note that $|\mathbf{Q}; \mathbf{p}\mathbf{q}\rangle$'s are orthonormal. Then we have

$$\langle \mathbf{Q}; \mathbf{p}\mathbf{q} | \frac{1}{z - H_0} | \mathbf{Q}; \mathbf{p}'\mathbf{q}' \rangle = G_0(\mathbf{Q}, z; \mathbf{p}\mathbf{q}) \delta_{\mathbf{p}, \mathbf{p}'} \delta_{\mathbf{q}, \mathbf{q}'}, \quad (2.14)$$

$$\langle \mathbf{Q}; \mathbf{p}\mathbf{q} | t_1(z) | \mathbf{Q}; \mathbf{p}'\mathbf{q}' \rangle = \frac{U}{N} \frac{1}{1 - UD_1(\mathbf{Q} + \mathbf{p}, z + \epsilon_{\mathbf{p}} - \mu)} \delta_{\mathbf{p}, \mathbf{p}'}, \quad (2.15)$$

$$\langle \mathbf{Q}; \mathbf{p}\mathbf{q} | t_2(z) | \mathbf{Q}; \mathbf{p}'\mathbf{q}' \rangle = \frac{-U}{N} \frac{1}{1 + UD_2(\mathbf{Q} - \mathbf{q}, z - \epsilon_{\mathbf{q}} + \mu)} \delta_{\mathbf{q}, \mathbf{q}'}, \quad (2.16)$$

with

$$D_1(\mathbf{k}, z) = \frac{1}{N} \sum_{\mathbf{q}'} \frac{1}{z - \epsilon_{\mathbf{k}-\mathbf{q}'} - Un - \epsilon_{\mathbf{q}'} + 2\mu}, \quad (2.17)$$

$$D_2(\mathbf{k}, z) = \frac{1}{N} \sum_{\mathbf{p}'} \frac{1}{z - \epsilon_{\mathbf{k}+\mathbf{p}'} - Un + \epsilon_{\mathbf{p}'}}. \quad (2.18)$$

For solving the Faddeev equation, we introduce the following quantities,

$$\Phi_{pp}(\mathbf{Q}, z; \mathbf{p}) = \sum_{\mathbf{p}'\mathbf{q}'} \langle \mathbf{Q}; \mathbf{p}\mathbf{q} | T_1(z) | \mathbf{Q}; \mathbf{p}'\mathbf{q}' \rangle G_0(\mathbf{Q}, z; \mathbf{p}'\mathbf{q}'), \quad (2.19)$$

$$\Phi_{ph}(\mathbf{Q}, z; \mathbf{q}) = \sum_{\mathbf{p}'\mathbf{q}'} \langle \mathbf{Q}; \mathbf{p}\mathbf{q} | T_2(z) | \mathbf{Q}; \mathbf{p}'\mathbf{q}' \rangle G_0(\mathbf{Q}, z; \mathbf{p}'\mathbf{q}'). \quad (2.20)$$

It will become clear below that Φ_{pp} is independent of \mathbf{q} and Φ_{ph} is independent of \mathbf{p} . Then the Faddeev equation is rewritten as

$$\begin{aligned} \Phi_{pp}(\mathbf{Q}, z; \mathbf{p}) &= \frac{UD_1(\mathbf{Q} + \mathbf{p}, z + \epsilon_{\mathbf{p}} - \mu)}{1 - UD_1(\mathbf{Q} + \mathbf{p}, z + \epsilon_{\mathbf{p}} - \mu)} \\ &+ \frac{U}{1 - UD_1(\mathbf{Q} + \mathbf{p}, z + \epsilon_{\mathbf{p}} - \mu)} \frac{1}{N} \sum_{\mathbf{q}'} G_0(\mathbf{Q}, z; \mathbf{p}\mathbf{q}') \Phi_{ph}(\mathbf{Q}, z; \mathbf{q}'), \end{aligned} \quad (2.21)$$

$$\begin{aligned} \Phi_{ph}(\mathbf{Q}, z; \mathbf{q}) &= \frac{-UD_2(\mathbf{Q} - \mathbf{q}, z - \epsilon_{\mathbf{q}} + \mu)}{1 + UD_2(\mathbf{Q} - \mathbf{q}, z - \epsilon_{\mathbf{q}} + \mu)} \\ &+ \frac{-U}{1 + UD_2(\mathbf{Q} - \mathbf{q}, z - \epsilon_{\mathbf{q}} + \mu)} \frac{1}{N} \sum_{\mathbf{p}'} G_0(\mathbf{Q}, z; \mathbf{p}'\mathbf{q}) \Phi_{pp}(\mathbf{Q}, z; \mathbf{p}'). \end{aligned} \quad (2.22)$$

An equation containing only $\Phi_{ph}(\mathbf{Q}, z; \mathbf{q})$ is obtained by substituting Eq. (2.21) into Eq. (2.22). This integral equation can be accurately solved for systems of fairly large size, since its variable is only \mathbf{q} for fixed \mathbf{Q} and z . Using the solution, we express the self-energy as

$$\Sigma_{\downarrow}(\mathbf{Q}, z) = \left(\frac{U}{N} \right)^2 \sum_{\mathbf{p}\mathbf{q}} G_0(\mathbf{Q}, z; \mathbf{p}\mathbf{q}) [1 + \Phi_{pp}(\mathbf{Q}, z; \mathbf{p}) + \Phi_{ph}(\mathbf{Q}, z; \mathbf{q})]. \quad (2.23)$$

There appear many poles determined from the condition $1 + UD_2(\mathbf{Q} - \mathbf{q}, z - \epsilon_{\mathbf{q}} + \mu) = 0$ in the low-energy region for the self-energy. They constitute a continuous spectrum in the single-particle spectra in the $N \rightarrow \infty$ limit. This condition is reduced to $z = \omega_{\mathbf{Q}-\mathbf{q}} + \epsilon_{\mathbf{q}} - \mu$ with $\omega_{\mathbf{k}}$ being the spin-wave energy in the random phase approximation (RPA). The lowest energy of the continuum spectra becomes zero at $\mathbf{Q} = \mathbf{k}_F$, since $\omega_0 + \epsilon_{\mathbf{k}_F} - \mu = 0$. For relatively small values of $|Q|$, bound states appear below the continuum. They are identified as “quasi-particles”, and their energy $E_{\mathbf{Q}}$'s are determined from

$$G(\mathbf{Q}, E_{\mathbf{Q}})^{-1} = E_{\mathbf{Q}} - [\epsilon_{\mathbf{Q}} - \mu + Un + \Sigma_{\downarrow}(\mathbf{Q}, E_{\mathbf{Q}})] = 0. \quad (2.24)$$

Now we comment on a widely used approximation called “ladder” approximation, which only considers the particle-particle ladder and particle-hole ladder separately. This is given by neglecting the second terms in Eqs. (2.21) and (2.22). As a results, the self-energy is given by

$$\Sigma_{\downarrow}(\mathbf{Q}, z) = U^2 \left\{ \frac{1}{N} \sum_{\mathbf{q}} \frac{D_2(\mathbf{Q} - \mathbf{q}, z - \epsilon_{\mathbf{q}} + \mu)}{1 + UD_2(\mathbf{Q} - \mathbf{q}, z - \epsilon_{\mathbf{q}} + \mu)} + \frac{1}{N} \sum_{\mathbf{p}} \frac{UD_1(\mathbf{Q} + \mathbf{p}, z + \epsilon_{\mathbf{p}} - \mu)^2}{1 - UD_1(\mathbf{Q} + \mathbf{p}, z + \epsilon_{\mathbf{p}} - \mu)} \right\}. \quad (2.25)$$

The first term comes from the particle-hole channel, which is interpreted as the electron-magnon interaction with bare vertex U . The second term comes from the particle-particle channel, and its contribution is much smaller than the first one in the strong coupling regime (except in the low density). As shown in the next section, the self-energy in this approximation is larger in order of magnitude than the present theory.

B. Limiting cases

We discuss several limiting cases for clarifying the physical meaning of the present theory.

1. Low density limit ($n \rightarrow 0$)

We expand the following quantities up to the first order of n :

$$\frac{-UD_2(\mathbf{Q} - \mathbf{q}, z - \epsilon_{\mathbf{q}} + \mu)}{1 + UD_2(\mathbf{Q} - \mathbf{q}, z - \epsilon_{\mathbf{q}} + \mu)} \approx \frac{-Un}{z - \epsilon_{\mathbf{Q}-\mathbf{q}} - \epsilon_{\mathbf{q}} + 2\mu}, \quad (2.26)$$

$$\frac{-U}{1 + UD_2(\mathbf{Q} - \mathbf{q}, z - \epsilon_{\mathbf{q}} + \mu)} \approx -U + \frac{U^2 n}{z - \epsilon_{\mathbf{Q}-\mathbf{q}} - \epsilon_{\mathbf{q}} + 2\mu}. \quad (2.27)$$

Substituting these relations into Eq. (2.22), we notice that the first term is order n and so is the second term, if $\Phi_{\text{pp}}(\mathbf{Q}, z; \mathbf{p})$ is order 1. Therefore we can neglect $\Phi_{\text{ph}}(\mathbf{Q}, z; \mathbf{q})$ in the lowest order of n , and thereby we obtain the lowest-order form of $\Phi_{\text{pp}}(\mathbf{Q}, z; \mathbf{p})$ as

$$\Phi_{\text{pp}}(\mathbf{Q}, z; \mathbf{p}) = \frac{UD_1(\mathbf{Q} + \mathbf{p}, z + \epsilon_{\mathbf{p}} - \mu)}{1 - UD_1(\mathbf{Q} + \mathbf{p}, z + \epsilon_{\mathbf{p}} - \mu)}. \quad (2.28)$$

Substituting this relation into Eq. (2.23) and using the relation $(1/N) \sum_{\mathbf{q}} G_0(\mathbf{Q}, z; \mathbf{p}\mathbf{q}) = D_1(\mathbf{Q} + \mathbf{p}, z + \epsilon_{\mathbf{p}} - \mu)$, we obtain in the lowest order

$$\begin{aligned} Un + \Sigma_{\downarrow}(\mathbf{Q}, z) &\approx \frac{1}{N} \sum_{\mathbf{p}} \frac{U}{1 - UD_1(\mathbf{Q} + \mathbf{p}, z + \epsilon_{\mathbf{p}} - \mu)} \\ &\approx \frac{Un}{1 - U \frac{1}{N} \sum_{\mathbf{q}'} \frac{1}{z - \epsilon_{\mathbf{Q}-\mathbf{q}'} - \epsilon_{\mathbf{q}'} + 2\mu}}. \end{aligned} \quad (2.29)$$

Here the chemical potential μ is located at the bottom of the band, so that \mathbf{q}' runs over the entire first Brillouin zone. This is nothing but the low-density expression Kanamori derived several decades ago.² Thus the present theory covers naturally the exact low-density limit.

2. Limit to the half-filling ($n \rightarrow 1$)

We expand the following quantities up to the first order of $1 - n$:

$$\frac{UD_1(\mathbf{Q} + \mathbf{p}, z + \epsilon_{\mathbf{p}} - \mu)}{1 - UD_1(\mathbf{Q} + \mathbf{p}, z + \epsilon_{\mathbf{p}} - \mu)} \approx \frac{U(1 - n)}{z - \epsilon_{\mathbf{Q}+\mathbf{p}-\mathbf{q}_0} + \epsilon_{\mathbf{p}} - U}, \quad (2.30)$$

$$\frac{U}{1 - UD_1(\mathbf{Q} + \mathbf{p}, z + \epsilon_{\mathbf{p}} - \mu)} \approx U + \frac{U(1 - n)}{z - \epsilon_{\mathbf{Q}+\mathbf{p}-\mathbf{q}_0} + \epsilon_{\mathbf{p}} - U}. \quad (2.31)$$

Here \mathbf{q}_0 stands for the momentum at the top of the valence band, *i. e.*, $\mathbf{q}_0 = (\pi, \pi)$ for the square lattice. Substituting these relations into Eq. (2.21), we notice that the first term becomes order $1 - n$ and so is the second term, if $\Phi_{\text{ph}}(\mathbf{Q}, z; \mathbf{q})$ is order 1. Therefore we can neglect $\Phi_{\text{pp}}(\mathbf{Q}, z; \mathbf{p})$ in the lowest order of $1 - n$, and thereby we obtain the lowest-order form of $\Phi_{\text{ph}}(\mathbf{Q}, z; \mathbf{q})$ as

$$\Phi_{\text{ph}}(\mathbf{Q}, z; \mathbf{q}) = \frac{-U \frac{1}{N} \sum_{\mathbf{p}'} \frac{1}{z - \epsilon_{\mathbf{Q}+\mathbf{p}'-\mathbf{q}_0} + \epsilon_{\mathbf{p}'} - U}}{1 + U \frac{1}{N} \sum_{\mathbf{p}'} \frac{1}{z - \epsilon_{\mathbf{Q}+\mathbf{p}'-\mathbf{q}_0} + \epsilon_{\mathbf{p}'} - U}}. \quad (2.32)$$

Substituting this relation into Eq. (2.23) and using a lowest-order relation $G_0(\mathbf{Q}, z; \mathbf{p}\mathbf{q}) \approx 1/[z - \epsilon_{\mathbf{Q}+\mathbf{p}-\mathbf{q}_0} + \epsilon_{\mathbf{p}} - U]$, we obtain up to the first order of $1 - n$

$$Un + \Sigma_{\downarrow}(\mathbf{Q}, z) \approx U - \frac{U(1 - n)}{1 + U \frac{1}{N} \sum_{\mathbf{p}'} \frac{1}{z - \epsilon_{\mathbf{Q}+\mathbf{p}'-\mathbf{q}_0} + \epsilon_{\mathbf{p}'} - U}}. \quad (2.33)$$

Here \mathbf{p}' runs over the entire first Brillouin zone.

Since available unoccupied states are limited in the up-spin band, the particle-particle multiple-scattering process gives rise to merely a higher-order contribution, in contrast to the low-density limit. Also, the processes creating more particle-hole pairs give rise to higher-order contributions. Thus Eq. (2.33) is exact up to the first order of $1 - n$ under the assumption of the saturated ferromagnetic ground state. But this expression is not so useful, since the saturated ferromagnetism is always unstable in this limit by the reason discussed below.

The second term of Eq. (2.33) vanishes as $n \rightarrow 1$, and one may think that the saturated ferromagnetic ground state is always stable around $n \sim 1$. This is not true, since the second term of Eq. (2.33) has a pole at $z = \omega_{\mathbf{Q}-\mathbf{q}_0}$, which is negative: $\Sigma_{\downarrow}(\mathbf{Q}, z) \propto 1/(z - \omega_{\mathbf{Q}-\mathbf{q}_0})$ for $z \sim \omega_{\mathbf{Q}-\mathbf{q}_0}$. Here $\omega_{\mathbf{k}}$ represents the RPA spin-wave energy at $n = 1$. Therefore $G_{\downarrow}(\mathbf{Q}, z)^{-1}$ can be zero for $z \sim \omega_{\mathbf{Q}-\mathbf{q}_0}$, even if $1 - n$ is very small. This means that the system is unstable through the coupling to the *unstable* spin-wave excitation. Figure 3 shows $\omega_{\mathbf{q}}$ for several values of U on the square lattice, demonstrating that it is always negative.

3. Atomic limit ($t \rightarrow 0$, $U < \infty$)

In the limit of $t \rightarrow 0$, we have

$$G_0(\mathbf{Q}, z; \mathbf{p}\mathbf{q}) \sim \frac{1}{z - Un}, \quad D_1(\mathbf{q}, z) \sim \frac{1 - n}{z - Un}, \quad D_2(\mathbf{q}, z) \sim \frac{n}{z - Un}. \quad (2.34)$$

Substituting these relations into Eqs. (2.21) and (2.22), we solve the Faddeev equation. The solution is given by

$$\Phi_{\text{pp}}(\mathbf{Q}, z; \mathbf{p}) \sim \frac{U(1 - n)}{z - U(1 - n)}, \quad \Phi_{\text{ph}}(\mathbf{Q}, z; \mathbf{q}) \sim \frac{-Un}{z - U(1 - n)}. \quad (2.35)$$

Substituting these relations into Eq. (2.23), we obtain the self-energy and the Green's function as

$$\Sigma_{\downarrow}(\mathbf{Q}, z) = U^2 \frac{n(1 - n)}{z - U(1 - n)}, \quad (2.36)$$

$$G_{\downarrow}(\mathbf{Q}, z) = \frac{1 - n}{z} + \frac{n}{z - U}. \quad (2.37)$$

This is the exact form in the atomic limit, first emphasized by Hubbard.¹ The fact that the three-body scattering approximation satisfies the exact atomic limit was first proved by one of the present author.⁶

4. Strong coupling limit ($U \rightarrow \infty$)

We expand $\Phi_{\text{pp}}(\mathbf{Q}, z; \mathbf{p})$ and $\Phi_{\text{ph}}(\mathbf{Q}, z; \mathbf{q})$ in powers of $1/U$,

$$\Phi_{\text{pp}}(\mathbf{Q}, z; \mathbf{p}) = \Phi_{\text{pp}}^{(0)}(\mathbf{Q}, z; \mathbf{p}) + \Phi_{\text{pp}}^{(1)}(\mathbf{Q}, z; \mathbf{p}) + \dots, \quad (2.38)$$

$$\Phi_{\text{ph}}(\mathbf{Q}, z; \mathbf{q}) = \Phi_{\text{ph}}^{(0)}(\mathbf{Q}, z; \mathbf{q}) + \Phi_{\text{ph}}^{(1)}(\mathbf{Q}, z; \mathbf{q}) + \dots. \quad (2.39)$$

Expanding also $D_1(\mathbf{k}, z)$ and $D_2(\mathbf{k}, z)$ in powers of $1/U$ and substituting them into Eqs. (2.21) and (2.22), we derive the equations for each order of $1/U$. The derivation of the solutions is straightforward but lengthy. We have summarized the derivation in the Appendix A, and here we simply show the result:

$$\Phi_{\text{pp}}^{(0)}(\mathbf{Q}, z; \mathbf{p}) = -1, \quad \frac{1}{N} \sum_{\mathbf{p}} \Phi_{\text{pp}}^{(1)}(\mathbf{Q}, z; \mathbf{p}) = -\frac{F(\mathbf{Q}, z)}{U}, \quad (2.40)$$

$$\Phi_{\text{ph}}^{(0)}(\mathbf{Q}, z; \mathbf{q}) = \frac{F(\mathbf{Q}, z)}{J(\mathbf{Q}, z; \mathbf{q})}, \quad \frac{1}{N} \sum_{\mathbf{q}} \Phi_{\text{ph}}^{(1)}(\mathbf{Q}, z; \mathbf{q}) = \frac{F(\mathbf{Q}, z)}{U}, \quad (2.41)$$

where

$$J(\mathbf{Q}, z; \mathbf{q}) = z - \epsilon_{\mathbf{q}} + \mu - \frac{1}{n} \frac{1}{N} \sum_{\mathbf{p}'} (\epsilon_{\mathbf{Q}+\mathbf{p}'-\mathbf{q}} - \epsilon_{\mathbf{p}'}), \quad (2.42)$$

$$F(\mathbf{Q}, z) = \frac{n}{\frac{1}{N} \sum_{\mathbf{q}} \frac{1}{J(\mathbf{Q}, z; \mathbf{q})}}. \quad (2.43)$$

Substituting these solutions into Eq. (2.23), and with the help of the expansion, $G_0(\mathbf{Q}, z; \mathbf{p}\mathbf{q}) \approx -[1/(Un) + (z - \epsilon_{\mathbf{Q}+\mathbf{p}-\mathbf{q}} - \epsilon_{\mathbf{q}} + \epsilon_{\mathbf{p}} + \mu)/(Un)^2]$, we obtain the self-energy

$$\Sigma(\mathbf{Q}, z) = -Un - F(\mathbf{Q}, z). \quad (2.44)$$

The first term cancels out the HF potential. This expression is different from the previously proposed one (Eq. (32) in Ref. 8). We verify numerically in the next section that the present expression gives the same quasi-particle energy as Roth's variational wave function.

C. Relation to the variational principle

We consider a system of N_e up-spin electrons and one down-spin electron with total momentum \mathbf{Q} . Let the wave function be

$$|\psi(\mathbf{Q})\rangle = \alpha|\mathbf{Q}\rangle + \sum_{\mathbf{p}\mathbf{q}} \beta_{\mathbf{p}\mathbf{q}}|\mathbf{Q}; \mathbf{p}\mathbf{q}\rangle. \quad (2.45)$$

Here $|\mathbf{Q}\rangle = a_{\mathbf{Q}\downarrow}^\dagger|F\rangle$, and $|\mathbf{Q}; \mathbf{p}\mathbf{q}\rangle$ was defined by Eq. (2.13), where \mathbf{p} and \mathbf{q} are restricted inside and outside the Fermi sphere in the up-spin band, respectively. Since the expectation value of energy E for this state is given by $E = \langle\psi|H|\psi\rangle/\langle\psi|\psi\rangle$, the extremum condition for E is reduced to the following eigenvalue equation:

$$\begin{aligned} H_{\mathbf{Q};\mathbf{Q}}\alpha + \sum_{\mathbf{p}\mathbf{q}} H_{\mathbf{Q};\mathbf{p}\mathbf{q}}\beta_{\mathbf{p}\mathbf{q}} &= E\alpha, \\ H_{\mathbf{p}\mathbf{q};\mathbf{Q}}\alpha + \sum_{\mathbf{p}'\mathbf{q}'} H_{\mathbf{p}\mathbf{q};\mathbf{p}'\mathbf{q}'}\beta_{\mathbf{p}'\mathbf{q}'} &= E\beta_{\mathbf{p}\mathbf{q}}, \end{aligned} \quad (2.46)$$

where $H_{\mathbf{Q};\mathbf{Q}} \equiv \langle\mathbf{Q}|H|\mathbf{Q}\rangle$, $H_{\mathbf{Q};\mathbf{p}\mathbf{q}} \equiv \langle\mathbf{Q}|H|\mathbf{Q}; \mathbf{p}\mathbf{q}\rangle$, $H_{\mathbf{p}\mathbf{q};\mathbf{Q}} \equiv \langle\mathbf{Q}; \mathbf{p}\mathbf{q}|H|\mathbf{Q}\rangle$, and $H_{\mathbf{p}\mathbf{q};\mathbf{p}'\mathbf{q}'} \equiv \langle\mathbf{Q}; \mathbf{p}\mathbf{q}|H|\mathbf{Q}; \mathbf{p}'\mathbf{q}'\rangle$. Instead of solving directly this eigenvalue problem, we calculate the resolvent $R(z) = 1/(z - H)$ by using the relation $R(z) \cdot (z - H) = 1$. It is given by

$$\langle\mathbf{Q}|R(z)|\mathbf{Q}\rangle = \left[z - H_{\mathbf{Q};\mathbf{Q}} - \sum_{\mathbf{p}\mathbf{q};\mathbf{p}'\mathbf{q}'} H_{\mathbf{Q};\mathbf{p}\mathbf{q}} S_{\mathbf{p}\mathbf{q};\mathbf{p}'\mathbf{q}'}(z) H_{\mathbf{p}'\mathbf{q}';\mathbf{Q}} \right]^{-1}, \quad (2.47)$$

where $S_{\mathbf{p}\mathbf{q};\mathbf{p}'\mathbf{q}'}(z) \equiv \langle\mathbf{Q}; \mathbf{p}\mathbf{q}|(z - H_3)^{-1}|\mathbf{Q}; \mathbf{p}'\mathbf{q}'\rangle$ with H_3 being the Hamiltonian operator represented by the components $\{H_{\mathbf{p}\mathbf{q};\mathbf{p}'\mathbf{q}'}\}$ within the three-body states. The Faddeev equation is one way of calculating $S_{\mathbf{p}\mathbf{q};\mathbf{p}'\mathbf{q}'}(z)$. Therefore, $\langle\mathbf{Q}|R(z)|\mathbf{Q}\rangle$ is essentially equivalent to $G(\mathbf{Q}, z)$ except for the origin of energy. Note that the poles of $R(z)$ give the energy eigenvalues, and let E_i 's be such energy eigenvalues. Then the excitation energies of overturning an up-spin electron at the Fermi level and placing it on a down-spin band are given by $E_i - \sum_{\mathbf{p}} \epsilon_{\mathbf{p}} - \mu$, which coincides with the energies of the poles of $G(\mathbf{Q}, z)$.

Now we compare the present theory with other variational theories. The variational wave function used by Roth^{16,18} is given by

$$|\Psi^R(\mathbf{Q})\rangle = \sum_i e^{i\mathbf{Q}\mathbf{r}_i} a_{i\downarrow}^\dagger \left(1 - \sum_j f(i-j) a_{j\uparrow}^\dagger a_{i\uparrow} \right) a_{\mathbf{k}_F\uparrow} |F\rangle, \quad (2.48)$$

where \mathbf{k}_F is a Fermi momentum, and $f(i-j)$ is the variational parameter. The total momentum of this state is $\mathbf{Q} - \mathbf{k}_F$. The wave function used by Shastry *et al.*²⁰ is given by putting $f(i-j) = \delta_{i,j}$ in Eq. (2.48). Roth's wave function neglects the correlation between the hole at the Fermi level (described by $a_{\mathbf{k}_F\uparrow}$) and other excitations. If this hole at the Fermi level is disregarded, Roth's wave function consists of three-body states of one particle-hole pair in the up-spin band and one electron in the down-spin band. Note that these states are limited in comparison with general three-body states, since two operators are confined on the same site i in Eq. (2.48). This restriction and the condition $f(0) = 1$ are necessary for avoiding the double occupancy in the $U = \infty$ limit. Therefore, we expect that the three-body scattering theory gives the same results as Roth's in the $U = \infty$ limit. Actually this is verified numerically in the next section. Recently, Hanish *et al.*²⁴ analyzed Roth's wave function on various lattices by using the resolvent method. They also extended Roth's wave function for finite U by including more doubly occupied states such as $a_{i\downarrow}^\dagger a_{i\uparrow}^\dagger a_{j\uparrow}$. Their method has an advantage of being able to treat systems of infinite size, but their wave function is still limited in comparison with the general three-body states, since two operators are still confined on the same site i . On this point, the three-body scattering theory remains superior to their approach.

III. CALCULATED RESULTS

Confining ourselves to finite systems of the square lattice, we calculate the single-particle Green's function. Since several $\epsilon_{\mathbf{k}}$'s are degenerate for finite systems, shell structures appear on physical quantities, depending on the occupation of up-spin electrons.^{15,16} The following numerical calculations are carried out on closed-shell configurations. We first eliminate $\Phi_{pp}(\mathbf{Q}, z; \mathbf{p})$ from Eqs. (2.21) and (2.22) to set up the integral equation for $\Phi_{ph}(\mathbf{Q}, z; \mathbf{q})$ only. Then we solve the equation on systems of finite size; the matrix of size $N(1-n) \times N(1-n)$ has to be inverted.

Figure 4 shows the quasi-particle energy and the lowest boundary of the continuum spectra as a function of \mathbf{Q} , for $\delta(\equiv 1-n) = 0.2$ and $4t/U = 0.05$. The calculation was carried out on a system of $N = 50 \times 50$ with a periodic boundary condition. The dispersion of the quasi-particle energy $E_{\mathbf{Q}}$ is extremely flat in comparison with a free dispersion $\epsilon_{\mathbf{Q}}$. The effective mass m^* is defined by $E_{\mathbf{Q}} = E_0 + (1/2m^*)Q^2$ around $\mathbf{Q} \sim 0$. The mass enhancement m^*/m (m is the free mass given by $\epsilon_{\mathbf{Q}}$) reaches to as large as 12 for this situation. The dispersion curve enters into the energy continuum for $Q_x = Q_y > 0.4\pi$. The quasi-particle peak may survive as a resonant peak after entering the continuum spectra. With increasing values of $|\mathbf{Q}|$, the boundary of the continuum spectra goes down and eventually touches to the x -axis at $\mathbf{Q} = \mathbf{k}_F$. A small gap seen at $\mathbf{Q} = \mathbf{k}_F$ in the figure is due to a finite-size effect.

Figure 5(a) shows the quasi-particle energy at $\mathbf{Q} = 0$, as a function of $4t/U$. The hole density and the system size are the same as in Fig. 4, $\delta = 0.2$ and $N = 50 \times 50$. The E_0 decreases with decreasing values of U . It turns negative for $4t/U > 0.085$, indicating that the Nagaoka ground state becomes unstable by overturning an up-spin electron at the Fermi level and placing it on the bottom of the down-spin band. Figure 5(b) shows E_0 evaluated in the ladder approximation. It is found that the first term in Eq. (2.25) has a dominant contribution. The absolute values are larger in order of magnitude than the values of the three-body scattering theory, suggesting that the ladder approximation overestimates the self-energy due to neglecting the vertex correction for the electron-magnon process. Note that the three-body scattering theory takes account of the vertex correction, since the *particle-hole* multiple-scattering process is renormalized by the *particle-particle* multiple-scattering process.

As already mentioned, the three-body scattering theory is expected to give the same quasi-particle energy as Roth's variational wave function in the $U = \infty$ limit. We demonstrate this equivalence in Fig. 6, which shows E_0 as a function of δ in comparison with the result of Roth's wave function.^{16,24} We have used Eq. (2.44) for the calculation on a system of size $N = 100 \times 100$. Both results coincide with each other within the accuracy of numerical errors.

Now we discuss the phase diagram for the Nagaoka ground state. We determine the phase boundary from the condition $E_{\mathbf{Q}} < 0$, which means the instability with respect to overturning an up-spin electron at the Fermi level and placing it on the down-spin band. Figure 7 shows the phase diagram thus evaluated in comparison with the results of other theories. Note that finite-size effects are not small even for relatively large size $N = 50 \times 50$. The solid line (SW) represents the boundary above which the energy of spin waves becomes negative within the RPA. The solid line (RR) represents the boundary determined by the method of Richmond and Rickayzen²³ (see Appendix B). The broken line represents the boundary given by Hanish *et al.* (the curve of "RES3" in Ref. 24).²⁶ All the curves have the similar slopes around $\delta \sim 0$, but depart from each other with increasing values of δ . The three-body scattering theory gives the most severe condition for the phase boundary, the smallest area of the Nagaoka state. The critical hole concentration is given by $\delta_c = 0.41$, the same as that of Hanish *et al.* This is reasonable since both theories become equivalent to using Roth's variational wave function in the $U = \infty$ -limit.

IV. CONCLUDING REMARKS

We have developed a many-body theory which takes account of the three-body multiple scattering, and have applied it to the two-dimensional Hubbard model by assuming the saturated ferromagnetic ground state. We have solved numerically the Faddeev equation of the three-body problem on systems of finite size, and have calculated the single-particle Green's function. We have found that the energy scale of the quasi-particle is smaller in order of magnitude than that of the ladder approximation. This difference comes from the lack of the vertex correction to the electron-magnon scattering process in the ladder approximation. Recently, a many-body theory called the fluctuation exchange approximation (FLEX)²⁷ is widely used in the paramagnetic phase. This is a self-consistent version of the ladder approximation, and has a nice feature of satisfying the conserving condition of Kadanoff and Baym.²⁸ One shortcoming of the FLEX is the lack of the vertex correction. For this reason, it may be interesting to extend the three-body scattering theory to the paramagnetic phase by setting up directly the integral equation instead of the Faddeev equation.

We have also studied the instability of the Nagaoka state. The present theory is regarded as a natural extension of Roth's variational wave function, having improved the phase diagram of the Nagaoka state. This result may serve as a measure of the accuracy of the present theory.

An accurate determination of the phase diagram is beyond the scope of this paper. If one uses more sophisticated variational wave functions, the area of the Nagaoka ground state can be reduced but remains finite. One of the best phase boundary was obtained by Wurth *et al.*,²⁹ who included more than 1000 terms with up to two particle-hole pair excitations in the variational calculation. Another interesting attempt was made by von der Linden and Edwards,¹⁶ who used the Slater determinant of the single-particle states of up-spin electrons influenced by the moving down-spin electron. The latter approach is regarded as an extension of the method of Richmond and Rickayzen.²³ Both gave smaller areas of the Nagaoka state than the present result. On the other hand, Davis and Feldkamp³⁰ pointed out that the method of Richmond and Rickayzen can be extended to calculate accurately the whole spectra of the single-particle excitations; one first diagonalize all ground and excited states in the presence of the static impurity of the down-spin electron and then diagonalize the hopping of the down-spin electron in this complete set of states. Of course the actual calculation has to be approximate by truncating the number of the excited states. Davis and Feldkamp³⁰ and one of the present authors⁷ applied this method to finite-size systems of the one-dimensional Hubbard model, and calculated the whole spectral function. This type of calculations has not been attempted yet on the two-dimensional Hubbard model.

So far, we have considered only the single-particle Green's function. The two-particle Green's function gives the poles of spin waves, whose softening may set another condition for the instability of the Nagaoka state. The phase diagram obtained by Okabe²² along this line is not better than the present one. As a natural extension of the present theory to calculate spin waves, we need to consider four-body correlations.

Finally we comment on the application to realistic situations of transition-metal compounds, in which five $3d$ -orbitals and the Hund-rule coupling are to be considered. The present theory is too complicated to treat such situations, and some simplifications have to be made. We have simplified the calculational scheme by using the local approximation. This type of calculations has been carried out for transition-metal mono-oxides³¹ and La_2CuO_4 and $\text{Sr}_2\text{CuO}_2\text{Cl}_2$,³² which improves considerably the single-particle spectra of the band calculation based on the local density approximation and leads to good agreement with the photoemission experiments.

ACKNOWLEDGMENTS

We would like to thank Dr. T. Okabe for valuable discussion. This work was partially supported by a Grant-in-Aid for Scientific Research from the Ministry of Education, Science, Sports and Culture, Japan.

APPENDIX A: DERIVATION OF EQS. (2.40) AND (2.41)

Expanding $D_1(\mathbf{k}, z)$ and $D_2(\mathbf{k}, z)$ in powers of $1/U$, we rewrite Eqs. (2.21) and (2.22) as

$$\begin{aligned} \Phi_{\text{pp}}(\mathbf{Q}, z; \mathbf{p}) = & -(1-n) - \frac{1-n}{U}(z + \epsilon_{\mathbf{p}} - \mu) + \frac{1}{U}A_{\text{pp}}(\mathbf{Q} + \mathbf{p}) + \cdots \\ & - \frac{1}{N} \sum_{\mathbf{q}'} \left\{ 1 + \frac{1}{U}(z + \epsilon_{\mathbf{p}} - \mu) - \frac{1}{Un}[\epsilon_{\mathbf{Q}+\mathbf{p}-\mathbf{q}'} + \epsilon_{\mathbf{q}'} - 2\mu - A_{\text{pp}}(\mathbf{Q} + \mathbf{p})] + \cdots \right\} \end{aligned}$$

$$\times \Phi_{\text{ph}}(\mathbf{Q}, z; \mathbf{q}'), \quad (\text{A1})$$

$$\begin{aligned} \Phi_{\text{ph}}(\mathbf{Q}, z; \mathbf{q}) &= \frac{-Un - (z - \epsilon_{\mathbf{q}} + \mu) + \frac{1}{n}A_{\text{ph}}(\mathbf{Q} - \mathbf{q})}{J(\mathbf{Q}, z; \mathbf{q})} + \frac{\frac{1}{n}A'_{\text{ph}}(\mathbf{Q} - \mathbf{q}, z)}{J(\mathbf{Q}, z; \mathbf{q})^2} + \dots \\ &+ \left\{ \frac{-1}{J(\mathbf{Q}, z; \mathbf{q})} + \frac{\frac{1}{Un^2}A'_{\text{ph}}(\mathbf{Q} - \mathbf{q}, z)}{J(\mathbf{Q}, z; \mathbf{q})^2} + \dots \right\} \\ &\times \frac{1}{N} \sum_{\mathbf{p}'} \left\{ U + \frac{z - \epsilon_{\mathbf{Q}+\mathbf{p}'-\mathbf{q}} - \epsilon_{\mathbf{q}} + \epsilon_{\mathbf{p}'} + \mu}{n} + \dots \right\} \Phi_{\text{pp}}(\mathbf{Q}, z; \mathbf{p}'), \end{aligned} \quad (\text{A2})$$

where

$$J(\mathbf{Q}, z; \mathbf{q}) = z - \epsilon_{\mathbf{q}} + \mu - \frac{1}{n}A_{\text{ph}}(\mathbf{Q} - \mathbf{q}), \quad (\text{A3})$$

$$A_{\text{pp}}(\mathbf{k}) = \frac{1}{N} \sum_{\mathbf{q}'} (\epsilon_{\mathbf{k}-\mathbf{q}'} + \epsilon_{\mathbf{q}'} - 2\mu), \quad (\text{A4})$$

$$A_{\text{ph}}(\mathbf{k}) = \frac{1}{N} \sum_{\mathbf{p}'} (\epsilon_{\mathbf{k}+\mathbf{p}'} - \epsilon_{\mathbf{p}'}), \quad (\text{A5})$$

$$A'_{\text{ph}}(\mathbf{k}, z) = \frac{1}{N} \sum_{\mathbf{p}'} (z - \epsilon_{\mathbf{k}+\mathbf{p}'} + \epsilon_{\mathbf{p}'})^2. \quad (\text{A6})$$

Then we expand $\Phi_{\text{pp}}(\mathbf{Q}, z; \mathbf{p})$ and $\Phi_{\text{ph}}(\mathbf{Q}, z; \mathbf{q})$ in powers of $1/U$ as written down in Eqs. (2.38) and (2.39). Substitute them into Eqs. (A1) and (A2) and arranging the terms in each order of $1/U$, we obtain the following relations:

$$0 = -\frac{Un}{J(\mathbf{Q}, z; \mathbf{q})} - \frac{U}{J(\mathbf{Q}, z; \mathbf{q})} \frac{1}{N} \sum_{\mathbf{p}'} \Phi_{\text{pp}}^{(0)}(\mathbf{Q}, z; \mathbf{p}'), \quad (\text{A7})$$

$$\Phi_{\text{pp}}^{(0)}(\mathbf{Q}, z; \mathbf{p}) = -(1-n) - \frac{1}{N} \sum_{\mathbf{q}'} \Phi_{\text{ph}}^{(0)}(\mathbf{Q}, z; \mathbf{q}'), \quad (\text{A8})$$

$$\begin{aligned} \Phi_{\text{ph}}^{(0)}(\mathbf{Q}, z; \mathbf{q}) &= -1 + \frac{1}{J(\mathbf{Q}, z; \mathbf{q})^2} \frac{1}{n} A'_{\text{ph}}(\mathbf{Q} - \mathbf{q}, z) \\ &- \frac{1}{nJ(\mathbf{Q}, z; \mathbf{q})} \frac{1}{N} \sum_{\mathbf{p}'} [z - \epsilon_{\mathbf{Q}+\mathbf{p}'-\mathbf{q}} - \epsilon_{\mathbf{q}} + \epsilon_{\mathbf{p}'} + \mu] \Phi_{\text{pp}}^{(0)}(\mathbf{Q}, z; \mathbf{p}') \\ &+ \frac{1}{n^2 J(\mathbf{Q}, z; \mathbf{q})^2} A'_{\text{ph}}(\mathbf{Q} - \mathbf{q}, z) \frac{1}{N} \sum_{\mathbf{p}'} \Phi_{\text{pp}}^{(0)}(\mathbf{Q}, z; \mathbf{p}') \\ &- U \frac{1}{J(\mathbf{Q}, z; \mathbf{q})} \frac{1}{N} \sum_{\mathbf{p}'} \Phi_{\text{pp}}^{(1)}(\mathbf{Q}, z; \mathbf{p}'), \end{aligned} \quad (\text{A9})$$

$$\begin{aligned} \Phi_{\text{pp}}^{(1)}(\mathbf{Q}, z; \mathbf{p}) &= -\frac{1-n}{U} (z + \epsilon_{\mathbf{p}} - \mu) + \frac{1}{U} A_{\text{pp}}(\mathbf{Q} + \mathbf{p}) \\ &- \frac{1}{U} \frac{1}{N} \sum_{\mathbf{q}'} \left[z + \epsilon_{\mathbf{p}} - \mu - \frac{1}{n} (\epsilon_{\mathbf{Q}+\mathbf{p}-\mathbf{q}'} + \epsilon_{\mathbf{q}'} - 2\mu - A_{\text{pp}}(\mathbf{Q} + \mathbf{p})) \right] \Phi_{\text{ph}}^{(0)}(\mathbf{Q}, z; \mathbf{q}') \\ &- \frac{1}{N} \sum_{\mathbf{q}'} \Phi_{\text{ph}}^{(1)}(\mathbf{Q}, z; \mathbf{q}'). \end{aligned} \quad (\text{A10})$$

Note that \mathbf{p}, \mathbf{p}' are restricted inside the Fermi sphere and \mathbf{q}, \mathbf{q}' are outside the Fermi sphere.

Equation (A8) indicates that $\Phi_{\text{pp}}^{(0)}(\mathbf{Q}, z; \mathbf{p})$ is independent of \mathbf{p} . This fact and Eq.(A7) leads to $\Phi_{\text{pp}}^{(0)}(\mathbf{Q}, z; \mathbf{p}) = -1$. Substituting this relation into Eqs. (A8) and (A9), we have

$$\frac{1}{N} \sum_{\mathbf{q}'} \Phi_{\text{ph}}^{(0)}(\mathbf{Q}, z; \mathbf{q}') = n, \quad (\text{A11})$$

$$\Phi_{\text{ph}}^{(0)}(\mathbf{Q}, z; \mathbf{q}) = -U \frac{1}{J(\mathbf{Q}, z; \mathbf{q})} \frac{1}{N} \sum_{\mathbf{p}'} \Phi_{\text{pp}}^{(1)}(\mathbf{Q}, z; \mathbf{p}'). \quad (\text{A12})$$

Here other terms in Eq. (A9) cancel out with each other. Equation (A12) indicates that the \mathbf{q} -dependence of $\Phi_{\text{ph}}^{(0)}(\mathbf{Q}, z; \mathbf{q})$ comes only from $J(\mathbf{Q}, z; \mathbf{q})$. Therefore $\Phi_{\text{ph}}^{(0)}(\mathbf{Q}, z; \mathbf{q})$ is written in a form

$$\Phi_{\text{ph}}^{(0)}(\mathbf{Q}, z; \mathbf{q}) = \frac{C}{J(\mathbf{Q}, z; \mathbf{q})}. \quad (\text{A13})$$

The constant C is determined by substituting Eq. (A13) into Eq. (A11):

$$C \equiv F(\mathbf{Q}, z) = \frac{n}{\frac{1}{N} \sum_{\mathbf{q}} \frac{1}{J(\mathbf{Q}, z; \mathbf{q})}}. \quad (\text{A14})$$

Substituting Eqs. (A13) into Eq. (A12), we obtain

$$\frac{1}{N} \sum_{\mathbf{p}'} \Phi_{\text{pp}}^{(1)}(\mathbf{Q}, z; \mathbf{p}') = -\frac{F(\mathbf{Q}, z)}{U}. \quad (\text{A15})$$

Next, we rewrite Eq. (A10) as

$$\begin{aligned} \Phi_{\text{pp}}^{(1)}(\mathbf{Q}, z; \mathbf{p}) &= -\frac{1}{Un} \sum_{\mathbf{q}'} (z - \epsilon_{\mathbf{Q}+\mathbf{p}-\mathbf{q}'} - \epsilon_{\mathbf{q}'} + \epsilon_{\mathbf{p}} + \mu) \Phi_{\text{ph}}^{(0)}(\mathbf{Q}, z; \mathbf{q}') \\ &\quad - \frac{1}{N} \sum_{\mathbf{q}'} \Phi_{\text{ph}}^{(1)}(\mathbf{Q}, z; \mathbf{q}'), \end{aligned} \quad (\text{A16})$$

with the help of Eq. (A11). Then we make sum with respect to \mathbf{p} in both sides of Eq. (A16). The first term on the right hand side satisfies the relation

$$\frac{1}{N} \sum_{\mathbf{p}} (z - \epsilon_{\mathbf{Q}+\mathbf{p}-\mathbf{q}'} - \epsilon_{\mathbf{q}'} + \epsilon_{\mathbf{p}} + \mu) \Phi_{\text{ph}}^{(0)}(\mathbf{Q}, z; \mathbf{q}') = nF(\mathbf{Q}, z), \quad (\text{A17})$$

which is independent of \mathbf{q}' . Using this relation, we have

$$\frac{1}{N} \sum_{\mathbf{p}'} \Phi_{\text{pp}}^{(1)}(\mathbf{Q}, z; \mathbf{p}') = -(1-n) \frac{F(\mathbf{Q}, z)}{U} - n \frac{1}{N} \sum_{\mathbf{q}'} \Phi_{\text{ph}}^{(1)}(\mathbf{Q}, z; \mathbf{q}'). \quad (\text{A18})$$

Substituting Eq. (A15) into this equation, we finally obtain

$$\frac{1}{N} \sum_{\mathbf{q}'} \Phi_{\text{ph}}^{(1)}(\mathbf{Q}, z; \mathbf{q}') = \frac{F(\mathbf{Q}, z)}{U}. \quad (\text{A19})$$

APPENDIX B: ADAPTION OF THE METHOD OF RICHMOND AND RICKAYZEN TO NUMERICAL CALCULATIONS

Consider the situation that there exist N_e up-spin electrons and one down-spin electron. Neglecting the kinetic energy for the down-spin electron, we assume that it sits at origin. The up-spin electrons are under the static repulsive potential localized at origin. Since there is no interaction working between up-spin electrons, we first calculate the single-particle energy by solving the potential problem, and then make N_e electrons occupy these energy levels according to the Pauli principle.

Let the wave functions of single particles be

$$|\psi^{(n)}\rangle = \sum_{\mathbf{k}} \alpha_{\mathbf{k}}^{(n)} |\mathbf{k}\rangle, \quad n = 1, 2, \dots, N, \quad (\text{B1})$$

where $|\mathbf{k}\rangle$ represents the normalized state of plane wave with wave vector \mathbf{k} . Then the energy eigenvalue $E^{(n)}$ is given by

$$\epsilon_{\mathbf{k}}\alpha_{\mathbf{k}}^{(n)} + \frac{U}{N} \sum_{\mathbf{k}'} \alpha_{\mathbf{k}'}^{(n)} = E^{(n)}\alpha_{\mathbf{k}}^{(n)}. \quad (\text{B2})$$

We solve numerically this equation by directly diagonalizing the corresponding matrix for systems of finite size (up to $N = 60 \times 60$), although it is also possible to solve it by using the Green's function. Lowest N_e levels are occupied by up-spin electrons, and thereby the energy of the system is given by

$$E_{\text{tot}} = \sum_{n=1}^{n=N_e} +E_{\downarrow}, \quad (\text{B3})$$

where $E_{\downarrow} = 0$, since we neglected the kinetic energy for down-spin electrons. The energy of the saturated ferromagnetic ground state for $N_e + 1$ up-spin electrons is given by $E_g^0 = \sum_{i=1}^{i=N_e+1} \epsilon_{\mathbf{k}_i}$. If E_{tot} is smaller than E_g^0 , the saturated ferromagnetic ground state is unstable.

- ¹ J. Hubbard, Proc. Royal Soc. London **A276**, 238 (1963).
- ² J. Kanamori, Prog. Theor. Phys. **30**, 275 (1963).
- ³ M. C. Gutzwiller, Phys. Rev. Lett. **10**, 159 (1963).
- ⁴ J. A. Hertz and D. M. Edwards, J. Phys. **F 3**, 2174 (1973); D. M. Edwards and J. A. Hertz, J. Phys. **F 3**, 2191 (1973).
- ⁵ H. Matsumoto, H. Umezawa, S. Seki, and M. Tachiki, Phys. Rev. **B 17**, 2276 (1978).
- ⁶ J. Igarashi, J. Phys. Soc. Jpn. **52**, 2827 (1983).
- ⁷ J. Igarashi, J. Phys. Soc. Jpn. **54**, 260 (1985).
- ⁸ A. E. Ruckenstein and S. Schmitt-Rink, Int. J. Mod. Phys. **B 3**, 1809 (1989).
- ⁹ The variational aspect of the three-body problem has discussed by E. G. Goryachev, Phys. Lett. **A 166**, 148 (1992).
- ¹⁰ T. C. Hsu and B. Doucot, Phys. Rev. **B 48**, 2131 (1993).
- ¹¹ Y. Nagaoka, Phys. Rev. **147**, 392 (1966).
- ¹² D. J. Thouless, Proc. Phys. Soc. **86**, 893 (1965).
- ¹³ Y. Fang, A. E. Ruckenstein, E. Dagotto and S. Schmitt-Rink, Phys. Rev. **B 40**, 7406 (1989).
- ¹⁴ B. Doucot and X. G. Wen, Phys. Rev. **B 40**, 2719 (1989).
- ¹⁵ A. Barbieri, J. A. Riera, and A. P. Young, Phys. Rev. **B 41**, 11697 (1990).
- ¹⁶ W. von der Linden and D. M. Edwards, J. Phys.: Cond. Matter **3**, 4917 (1991).
- ¹⁷ J. Hirsch, Phys. Rev. **B 31**, 4403 (1985).
- ¹⁸ L. M. Roth, Phys. Chem. Solids **28**, 1549 (1967); Phys. Rev. **186**, 428 (1969).
- ¹⁹ S. R. Allan and D. M. Edwards, J. Phys. **F 12**, 1203 (1982).
- ²⁰ B. S. Shastry, H. R. Krishnamurthy and P. W. Anderson, Phys. Rev. **B 41**, 2375 (1990).
- ²¹ A. G. Basile and V. Elser, Phys. Rev. **B 41**, 4842 (1990).
- ²² T. Okabe, Prog. Theor. Phys. **97**, 21 (1997); Phys. Rev. **B 57**, 403 (1998).
- ²³ P. Richmond and R. Rickayzen, J. Phys. **C 2**, 528 (1969).
- ²⁴ T. Hanish, G. S. Uhlig and E. Müller-Hartmann, Phys. Rev. **B 56**, 13960 (1997).
- ²⁵ L. D. Faddeev, Zh. Eksperim. Teor. Fiz. **39**, 1459 (1960) [English transl.:Soviet Phys.-JETP **12**, 1014 (1961)].
- ²⁶ This curve is very close to that of Roth's wave function. See also the curve "RES2" in Ref. 24.
- ²⁷ N. E. Bickers and D. J. Scalapino, Annals of Physics, **193**, 206 (1989).
- ²⁸ L. P. Kadanoff and G. Baym, *Quantum Statistical Mechanics* (Benjamin, Menlo Park, 1962).
- ²⁹ P. Wurth, G. S. Uhrig and Müller-Hartmann, Ann. Phys. (Leipzig) **5**, 148 (1996).
- ³⁰ L. C. Davis and L. A. Feldkamp, J. Appl. Phys. **50**, 1944 (1979).
- ³¹ M. Takahashi and J. Igarashi, Ann. Phys. (Leipzig) **5**, 247 (1996); Phys. Rev. **B 54**, 13566 (1996); Phys. Rev. **B 56**, 12818 (1997).
- ³² M. Takahashi and J. Igarashi, Phys. Rev. **B 59**, (1999) No.11.

FIG. 1. Feynman diagrams for the self-energy $\Sigma_{\downarrow}(\mathbf{Q}, z)$ within the three-body scattering theory. Only three lines of Green's functions exist in the intermediate states. The broken lines represent the Coulomb interaction.

FIG. 2. A sketch for a three-body state $|\mathbf{Q}; \mathbf{p}\mathbf{q}\rangle$.

FIG. 3. Dispersion of spin-wave energy $\omega_{\mathbf{q}}$ along the line from $\mathbf{q} = (0,0)$ to (π,π) within the RPA. The density of up-spin electrons is $n = 1$, and the system size is $N = 100 \times 100$.

FIG. 4. Quasi-particle energy $E_{\mathbf{Q}}$ and the lowest boundary of the continuum spectra as a function of \mathbf{Q} . The calculation is carried out for a system of $N = 50 \times 50$. The hole density and the Coulomb interaction are $\delta (= 1 - n) = 0.2$ and $4t/U = 0.05$, respectively.

FIG. 5. Quasi-particle energy $E_{\mathbf{Q}}$ at $\mathbf{Q} = 0$ as a function of $4t/U$. The hole density is $\delta = 0.2$ and the system size is $N = 50 \times 50$; (a) the three-body scattering theory; (b) the ladder approximation. The line with lower energy in (b) is the contribution only from the first term of Eq. (2.25).

FIG. 6. Quasi-particle energy $E_{\mathbf{Q}}$ at $\mathbf{Q} = 0$ as a function of δ in the $U = \infty$ limit. The system size is $N = 100 \times 100$. The solid line represents the result of Roth's wave function (taken from Fig. 1 in Ref. 24).

FIG. 7. Phase diagram for the square lattice. Open circles are for a system of $N = 40 \times 40$, and the solid squares are for a system of $N = 50 \times 50$. The broken line is the curve "RES3" of Hanisch *et al.*²⁴. The solid line with letters "SW" represents the boundary above which the instability of the RPA spin-waves become unstable. The solid line with letters "RR" represents the boundary given by the method of Richmond and Rickayzen.

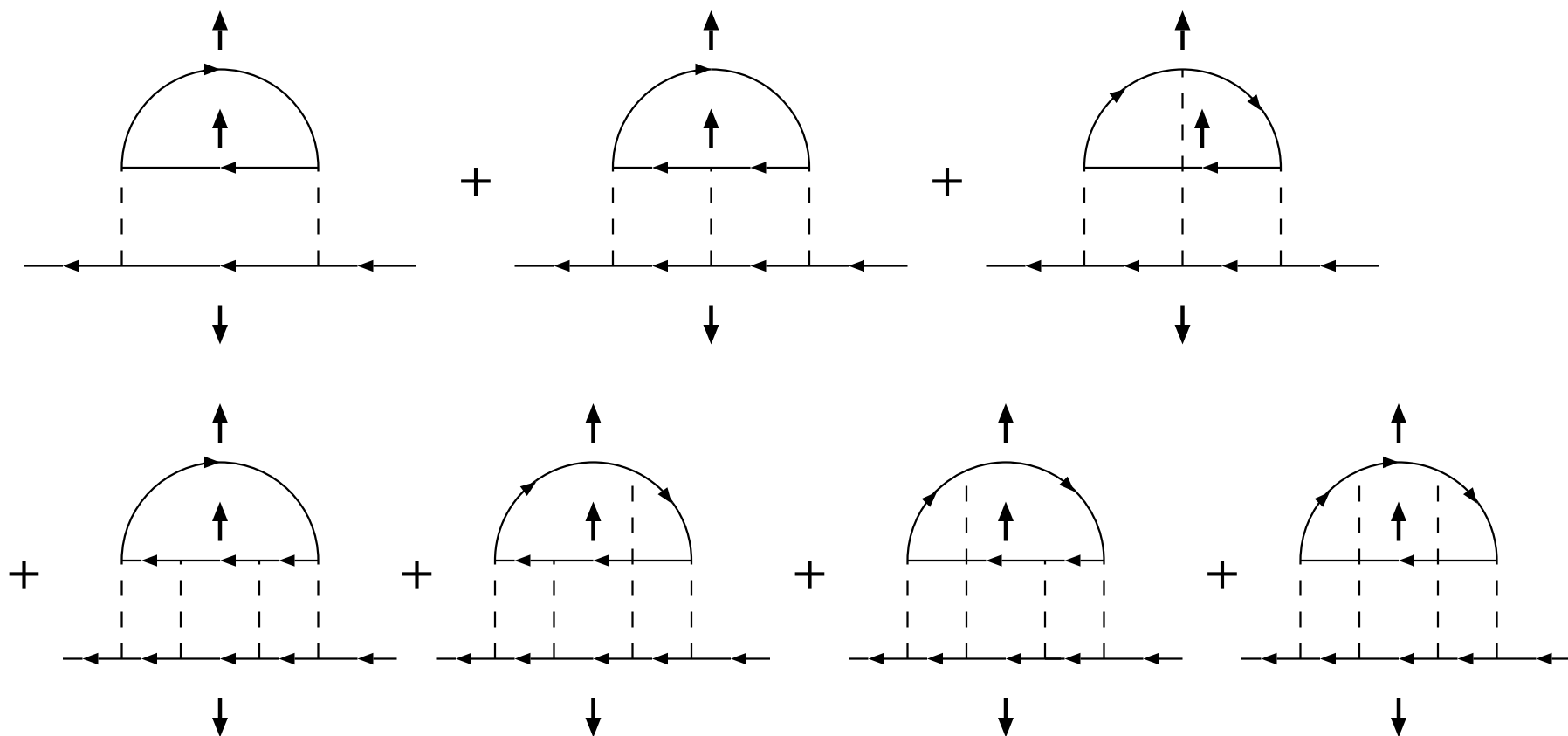


Fig. 1

J. Igarashi, M. Takahashi & T. Nagao

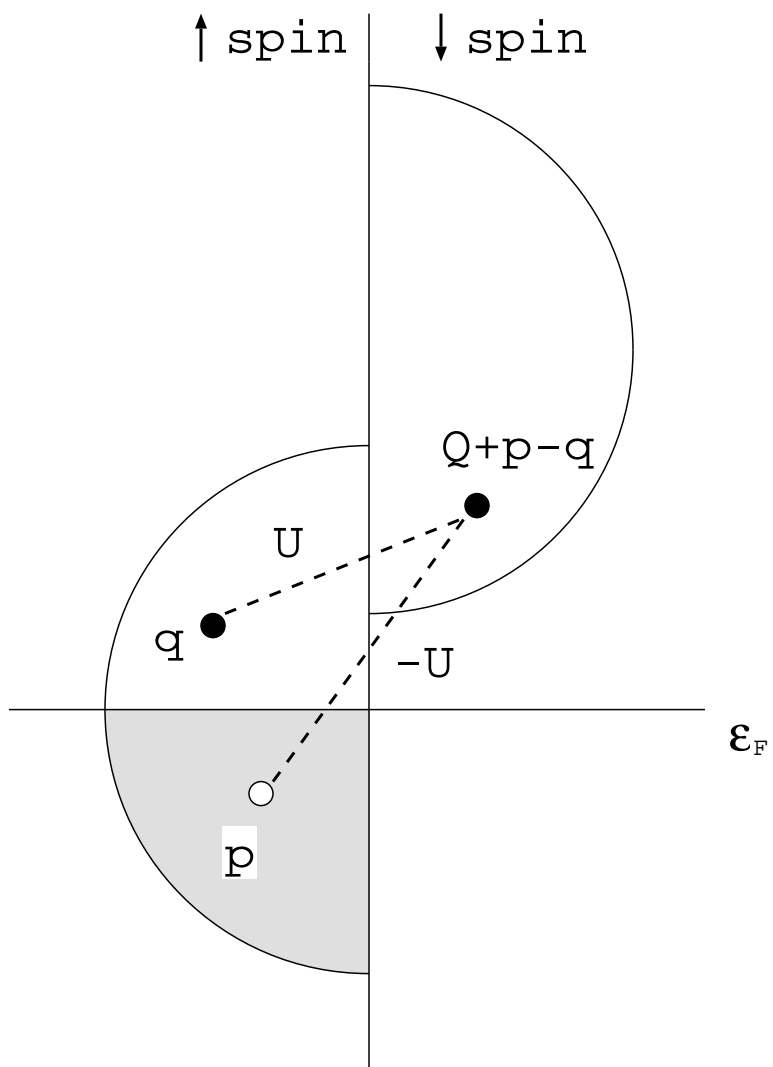


Fig. 2

J.Igarashi, M.Takahashi & T.Nagao

Fig. 3

J. Igarashi, M. Takahashi & T. Nagao

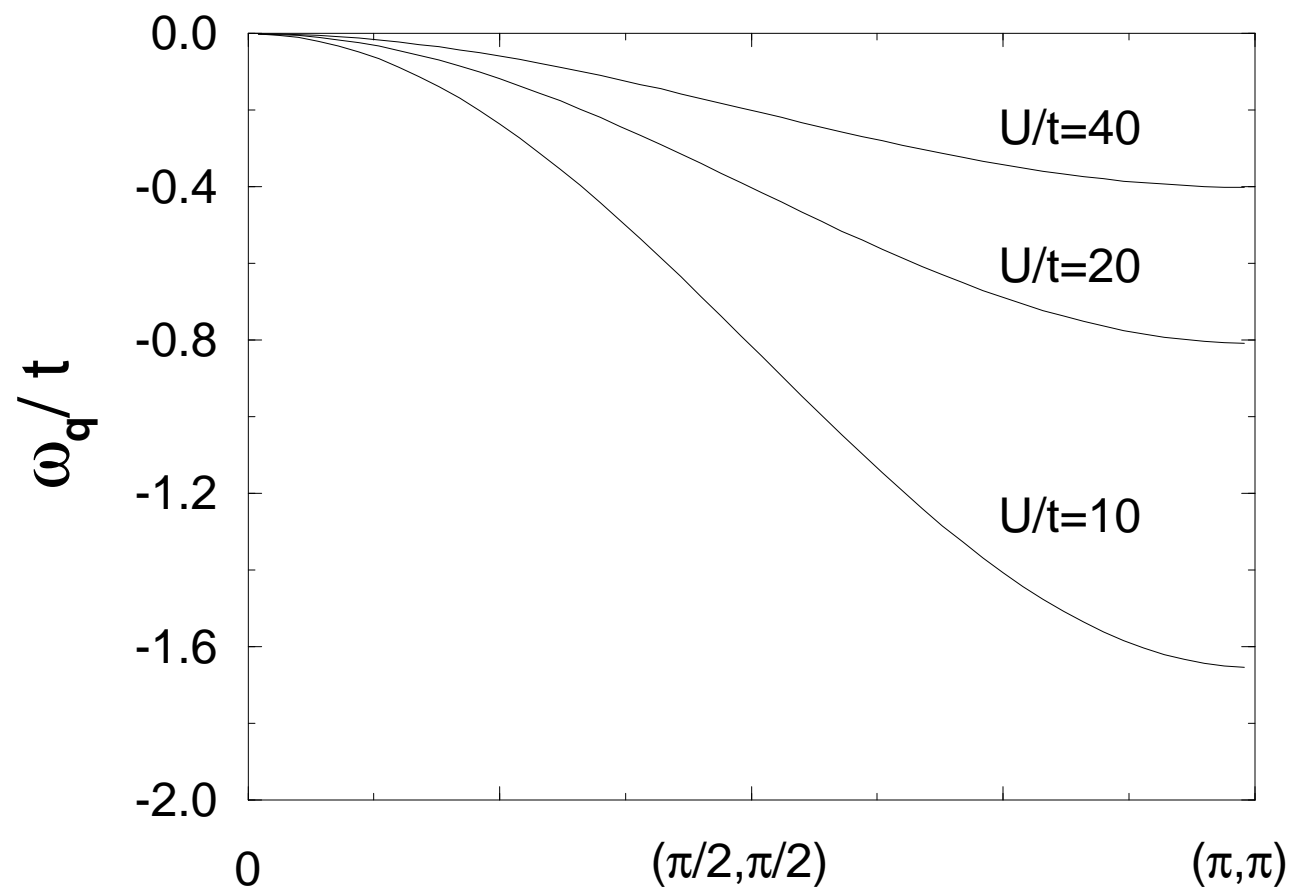


Fig. 4

J. Igarashi, M. Takahashi & T. Nagao

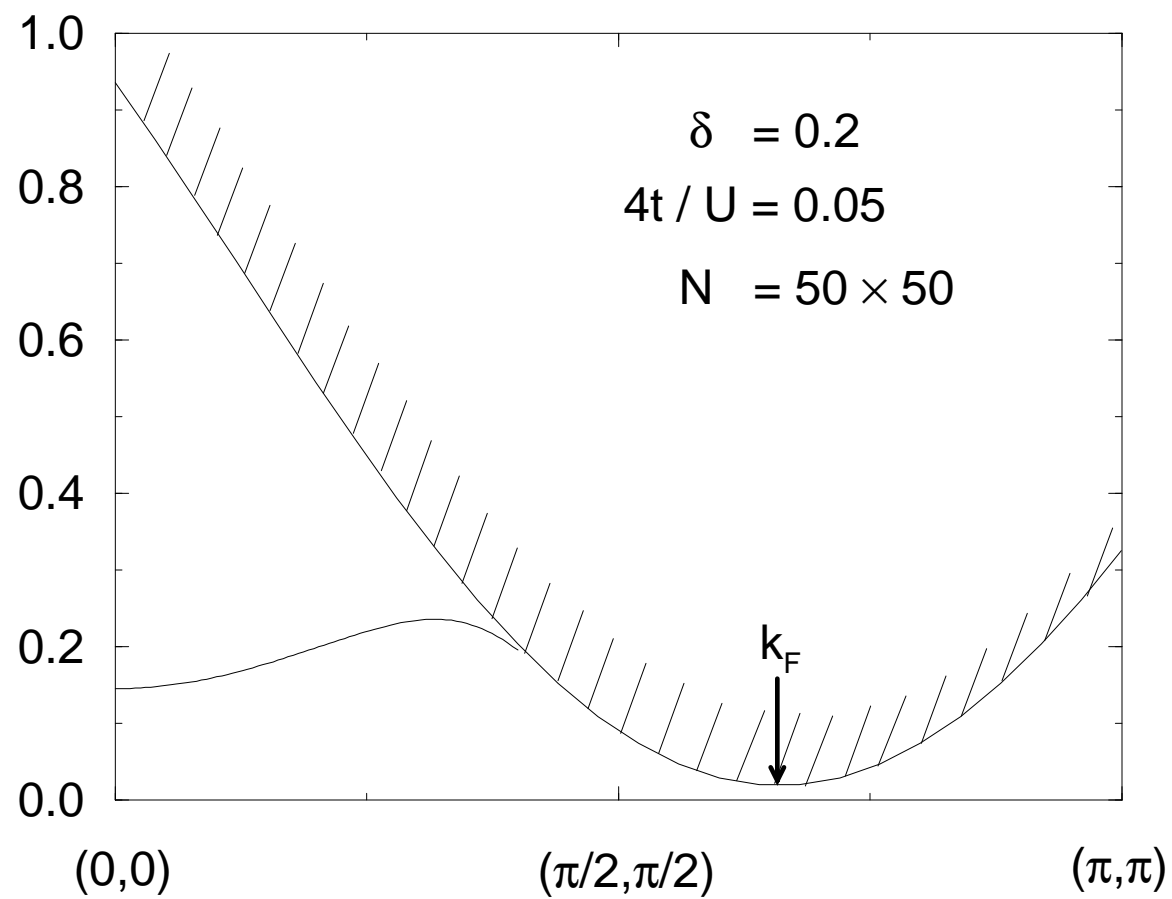


Fig. 5 (a)

J. Igarashi, M. Takahashi & T. Nagao

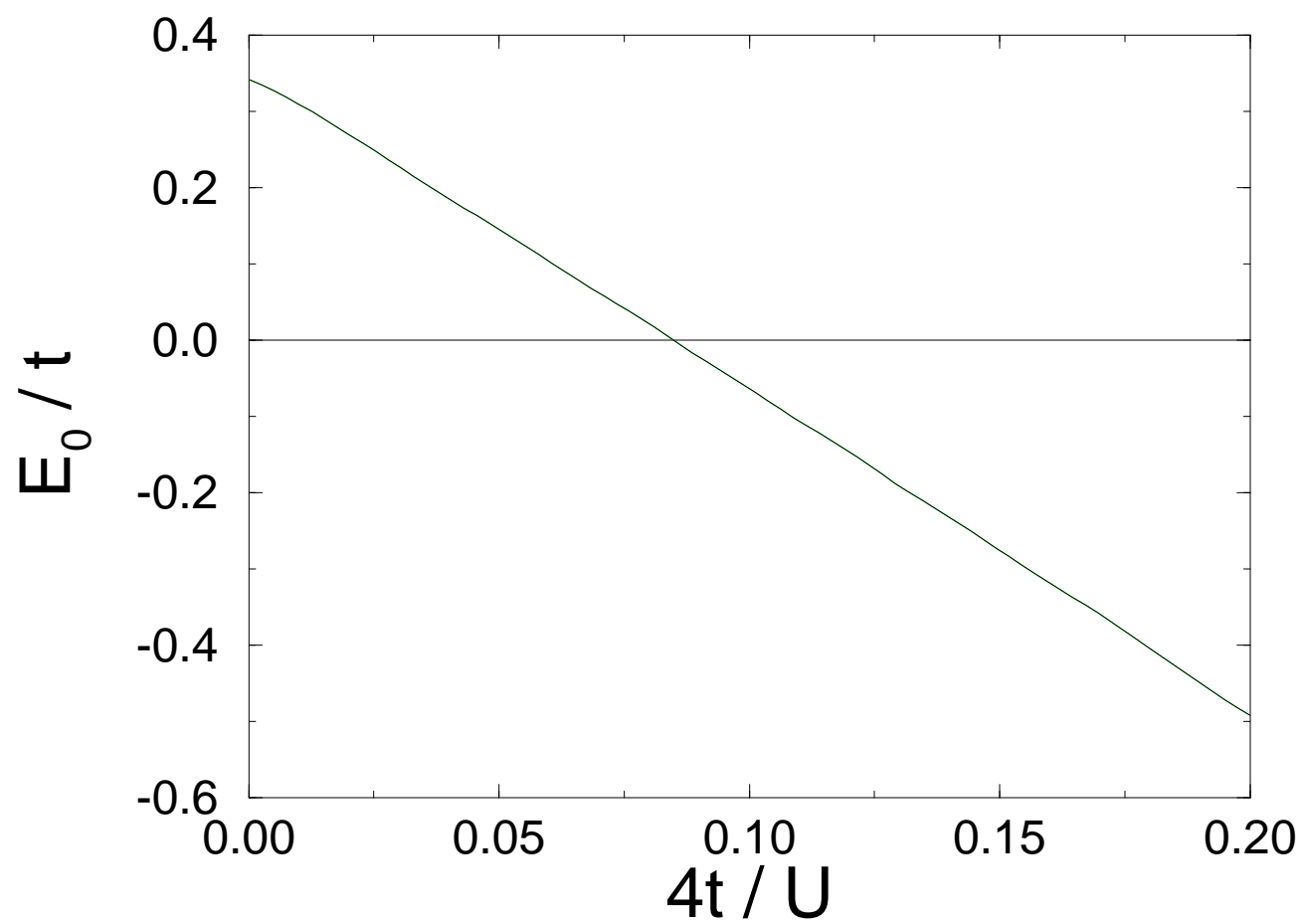


Fig. 5 (b)

J. Igarashi, M. Takahashi & T. Nagao

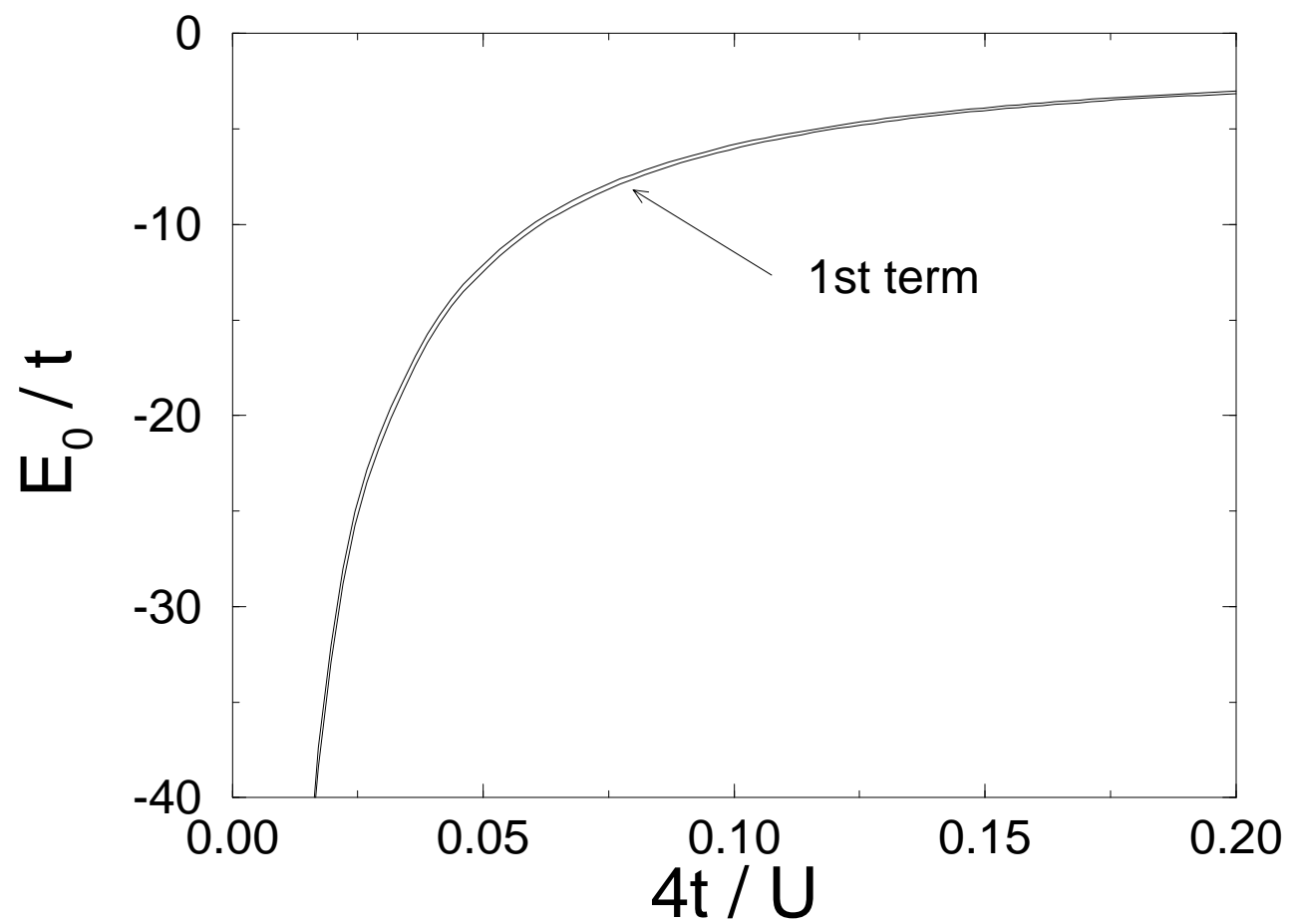


Fig. 6

J. Igarashi, M. Takahashi & T. Nagao

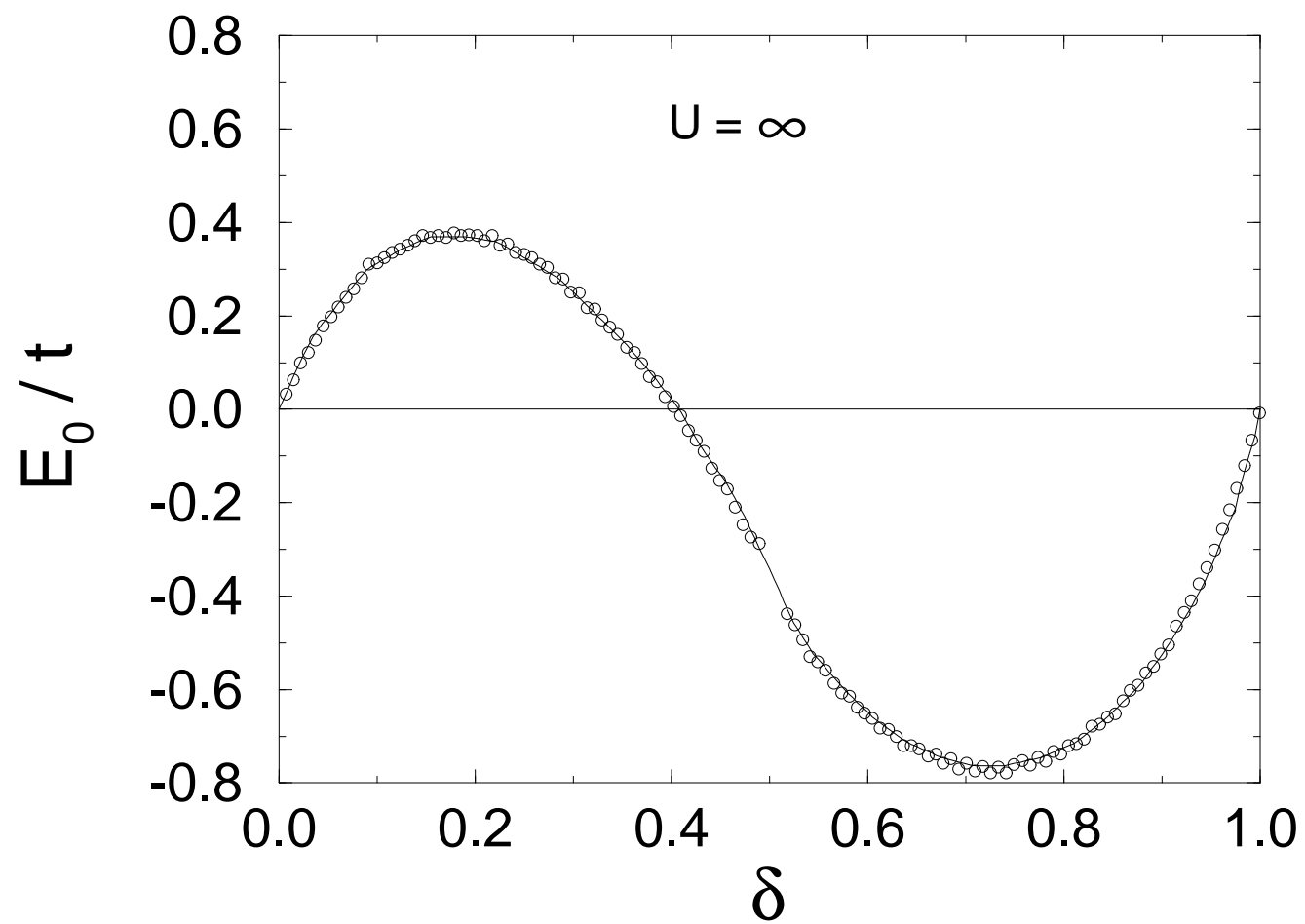


Fig. 7

J. Igarashi, M. Takahashi & T. Nagao

